APPLICATION OF THE PADÉ APPROXIMANT METHOD TO AN INVESTIGATION OF THE SUSCEPTIBILITY OF AN ISING SQUARE LATTICE *

A. V. FERRIS-PRABHU
NASA Goddard Space Flight Center, Greenbelt, Maryland

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Methods of calculating spin-spin correlation functions have been proposed by Clapp [1] to determine various thermodynamic properties of magnetic systems. Based on his exact cluster, and self-consistent method calculations, the Padé technique was applied to determine the location and nature of the singularity in the susceptibility of an Ising square lattice.

Fisher [2] gives the following high temperature formula

$$\chi = \frac{N\mu^2}{kT} \sum_{n=0}^{N} \langle \sigma_0^z \sigma_n^z \rangle : T > T_c \qquad (1)$$

where χ is the susceptibility, N the number of spins in the system, μ the magnetic moment of each spin, k the Boltzmann constant, T the absolute temperature and $\langle \sigma_0 \sigma_n \rangle$ the correlation function for the z components of the spin. $\sigma = 2S + \frac{1}{2}$ here.

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Eq. (1) may be rewritten [1] as

$$\chi = \frac{N\mu^2}{3kt} \frac{3+4t^2-4t^4}{1-2\langle 01\rangle/(1+2t^2-2t^4)} \qquad (2)$$

where $t = \tanh \frac{1}{2}\beta J$, $\beta = 1/kT$, J is the exchange integral and $\langle 01\rangle$ the correlation function, is a ratio of two polynomials in t. The effect of the number of spins in the cluster enters through these polynomials, and $\langle 01\rangle$ has been tabulated [1] for several clusters. Eq. (2) easily reduces to

$$\chi = A(t)/B(t)$$

where $A(t)$, $B(t)$ are polynomials in t. The Padé technique [3] is now applicable. The smallest real positive value of t for which the denominator of the logarithmic derivative of the susceptibility is zero locates the critical point, and the residue there gives the power with which the susceptibility diverges. The results of an IBM 709 program to calculate this is given in table 1.

Table 1

No. of spins in cluster	6	9	20	25	30
t_c	0.521	0.473	0.442	*	0.431

* This value was lost.

In each case the residue is -1 implying that for this model the susceptibility diverges as $1/(t-t_c)$. The value of the critical temperature decreases as the cluster size increases and for an infinitely large cluster it might converge to Onsager's exact value of 0.414 [4].

The self consistent method [1] gives excellent results and is briefly described.

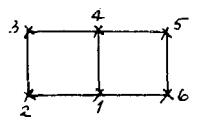

Fig. 1.

In fig. 1 the bonds represent the exchange coupling between spins located on the numbered sites. The coupling between spins 1 and 4 is assumed to have a constant value J. All other couplings are assumed to have a temperature dependent value $J_1(T)$ which is determined by requiring that at all temperatures the correlations between spins 1 and 4 and any outside nearest neighbor pair be equal. This is plausible because in an infinite lattice of which this cluster is a part, a spin pair like 1-2 will have coupling paths in the rest of the lattice in addition to those in the cluster. If this temperature dependent coupling be represented by $J'(T)$ then the effective coupling will be given by $J_1(T)$, i.e., by $J + J'$. For an inner pair like 1-4, it is assumed that the coupling from the rest of the lattice is accounted for by the augmented coupling between the spins on the perimeter of the cluster, enabling the coupling to be kept at the constant value J.

Thus, the correlation function $\langle 01\rangle$ which is a function of J and J_1 appears as a ratio of polynomials in t and t_1 ($t_1 = \tanh \frac{1}{2}\beta J_1$). The requirement that in an infinite crystal all nearest neighbor correlation functions be equal leads to the self consistency relation $t_1 = (1-\sqrt{1-4t^2})/2t$. Eq. (2) then reduces to the form

$$\chi = \frac{A(t,t_1)}{B(t,t_1)} = \frac{\sum A_n t^n}{\sum B_n t^n} = \sum Q_n t^n$$

where t_1 is replaced by its series expansion in t where the coefficients were computed on an IBM 709.

The Padé technique is particularly suitable here. The first twenty Padé approximants to the logarithmic derivative of the susceptibility were calculated and their poles located. The smallest real positive value of t for which a pole occurred was identified as t_c, and the residue was evaluated at t_c. The results are given in table 2.

Table 2

N	t_c	Residue
1	0.83333333	- 4.61
2	0.8259	- 3.59
3	0.3467212	- 0.336211
4	0.4072426	- 0.793024
5	0.4151549	- 0.915533
6	3.4049675	33.771
7	0.41884024	- 1.00726
8	0.41859223	- 0.998611
9	0.41862295	- 0.999777
10	0.41862277	- 0.999769
11	0.41862652	- 0.999937
12	0.41862779	- 1.00000
13	0.41862779	- 1.00000
14	0.41862778	- 1.00000
	0.21132568 *	-11.3761×10^{-7} *
15	0.41862864	- 1.00000
16	0.41862795	- 1.00004
17	0.41862788	- 1.00001
18	0.41862784	- 1.00001
19	0.41862816	- 1.00001
20	0.41862770	- 1.00002

* The first pole occurs here

The fifth approximant locates t_c at 0.4151549 which is in excellent agreement with Onsager's value of 0.414. The sixth approximant behaves strangely with t_c at 3.4049675 and a residue of 33.771. This result seems spurious though it is not clear why it appears. The next fourteen approximants behave well and t_c converges rapidly to 0.41862770 with a slight oscillation in the last two decimal places. The residue rapidly becomes -1.

Though the behaviour of the susceptibility at the critical point is not accurately predicted by [1], yet the Padé technique locates the critical temperature excellently. Calculations are in progress to apply the Padé technique to locate the singularity in the specific heat of an Ising lattice and the susceptibility and specific heat of a Heisenberg lattice.

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